Single-copy entanglement in critical quantum spin chains

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We introduce the single-copy entanglement as a quantity to assess quantum correlations in the ground state in quantum many-body systems. We show for a large class of models that already on the level of single specimens of spin chains, criticality is accompanied with the possibility of distilling a maximally entangled state of arbitrary dimension from a sufficiently large block deterministically, with local operations and classical communication. These analytical results – which refine previous results on the divergence of block entropy as the rate at which EPR pairs can be distilled from many identically prepared chains, and which apply to single systems as encountered in actual experimental situations – are made quantitative for general isotropic translationally invariant spin chains that can be mapped onto a quasi-free fermionic system, and for the anisotropic XY model. For the XX model, we provide the asymptotic scaling of $\sim (1/6)\log_2(L)$, and contrast it with the block entropy. The role of superselection rules on single-copy entanglement in systems consisting of indistinguishable particles is emphasized.

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Quantum phase transitions of second order are accompanied with a divergent length scale: this is the classical correlation length, the characteristic length associated with the two-point correlation function [1]. Recently, it has increasingly become clear that one should expect additional insight in the scaling of quantum correlations present in the ground state of a many-body system at or close to a quantum phase transition by expressing them in terms of entanglement properties [2, 3, 4, 5, 6, 7, 8, 9, 10, 12]. Entanglement, after all, plays a fundamental role in quantum phase transitions at zero temperature. The theory of entanglement in turn – developed in the quantum information context – provides tools to characterize and quantify genuine quantum correlations in contrast to correlations that occur in states that can be prepared with mere local preparations together with classical communication (LOCC). In particular, one finds that in one-dimensional non-critical harmonic [3, 4, 5] or quantum spin systems [5, 6, 7, 8, 9], the degree of entanglement of a block of L systems, quantified in terms of the entropy of the reduction, typically saturates for large block size, with higher-dimensional "entropy-area laws" [4]. In contrast, in critical spin systems or in fermionic systems, the entropy of a reduction has logarithmic corrections as $L \to \infty$ [6, 7, 8, 10]. These findings are consistent with expectations from conformal field theory [5]. Such a behavior of the block entropy has also been related to the performance of DMRG simulations of ground state properties. This von-Neumann entropy of a block quantifies the rate at which one can asymptotically distill maximally entangled qubit pairs under LOCC, when one has infinitely many identically prepared many-body systems at hand [11].

Yet, in several contexts, in particular for condensed-matter systems, this asymptotic notion of entanglement implicitly referring to joint operations on many identical systems may not always be the most appropriate one. Instead, one may ask: *does a single specimen of a critical infinite system already contain an infinite amount of entanglement*? This will be the central question of this paper. We introduce the single-copy entanglement to quantify the quantum correlations in critical and non-critical many-body systems. More specifically, compared to the divergence of the block entropy, we ask the stronger question whether a single spin chain already contains an arbitrary amount of entanglement, such that from a single specimen a maximally entangled state of arbitrary dimension can be distilled.

We will make the argument quantitative by analytically considering a general framework of translationally invariant quantum spin models. As examples in which criticality is in one-to-one correspondence with a divergent single-copy entanglement, we consider isotropic spin models, as well as the XY-model. For the isotropic XY model we establish the exact asymptotic scaling behavior of $\sim (1/6)\log_2(L)$, and relate it to the block entropy [7, 8]. The results can also be conceived as statements concerning the divergence of fine-grained entanglement [12].

Single-copy entanglement. – Let us consider a one-dimensional quantum spin system, associated with a Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$, with a translationally invariant Hamiltonian. We distinguish a block of length L of consecutive systems of the chain. So we have a bi-partioning $n|L$, the whole system being in a pure state $\rho = |\psi\rangle\langle\psi|$.

There are several meaninful definitions of single-copy entanglement. We will primarily be concerned with the question: running a physical device once, a maximally entangled state of what dimension can be distilled from a single specimen with certainty? Hence, the state has a single-copy entanglement $E_1(\rho) = \log_2(M)$, with respect to the bi-partitioning $n|L$, if ρ can be deterministically transformed under LOCC into $|\psi_M\rangle\langle\psi_M|$, i.e., a maximally entangled state with state vector $|\psi_M\rangle = (|1,1\rangle + ... + |M,M\rangle)/\sqrt{M}$, so if

$$\rho \longrightarrow |\psi_M\rangle\langle\psi_M| \text{ under LOCC.} \tag{1}$$

This is the non-asymptotic analogue of the entropy of entanglement of the reduction associated with a block of length L.

Denote with $\alpha_1^{\downarrow}, ..., \alpha_{2^L}^{\downarrow}$ the non-increasingly ordered eigenvalues of the reduced state with respect to a block of length L, then Eq. (1) holds true if and only if [13] $\sum_{k=1}^{K} \alpha_k^{\downarrow} \leq K/M$ for all $1 \leq K \leq M$, so obviously, if and only if $\alpha_1^{\downarrow} \leq 1/M$. In other words, the transformation is possible if the reduction is more mixed in the sense of majorization than the reduction of the maximally entangled state of dimension $M \times M$. Given $\alpha_1^{\downarrow}$, the single-copy entanglement is nothing but $E_1(\rho) = \log_2(\lfloor (\alpha_1^{\downarrow})^{-1} \rfloor)$. A variant is one allowing for probabilistic protocols. For a state ρ we say that

$$E_{\mathrm{p}}(\rho) = \sup \sum_{k=0}^{\infty} p_k \log_2(M_k),$$

such that ρ can be transformed under LOCC into the ensemble $\{(p_k, |\psi_{M_k}\rangle\langle\psi_{M_k}|) : k = 0, 1, ...\}$. This is the average entanglement that can be distilled, allowing for maximally entangled states of different dimension with certain probabilities [14]. This rate is then the solution of a linear program [16]. By definition, we have that $E_1(\rho) \leq E_{\mathrm{p}}(\rho) \leq S(\mathrm{tr}_{n\setminus L}[\rho])$, where the last inequality follows from the fact that the entropy of a reduction bounds the rate of any (asymptotic) distillation protocol.

Finally, note that for the single-copy entanglement, superselection rules (SSR) play a crucial role, notably a SSR with respect to particle number conservation. In the presence of SSR, E_1^{SSR} has to be understood as referring to a probabilistic transformation distilling entanglement-EPR states with state vector $|\psi^{\mathrm{SSR}}\rangle = (|0,1\rangle|1,0\rangle + |1,0\rangle|0,1\rangle)/\sqrt{2}$ under LOCC and SSR. We will now consider the behavior of the single-copy entanglement in the limit of large L for critical and non-critical spin chains.

Single-copy entanglement in general quantum spin chains. – We start from the general set of translationally invariant quantum spin systems that is as in Ref. [8] mapped onto a fermionic quadratic Hamiltonian under a Jordan-Wigner transformation. This model embodies a large class of spin models, including the anisotropic and isotropic XY-models as important special cases. Hence, the Hamiltonian is

$$H = \sum_{q=0,1} \sum_{k,j=1}^{n} \left(\frac{B_{j-k}}{2} - \frac{A_{j-k}}{4} \right) \hat{\sigma}_k^{q+1} \Bigg[\prod_{\substack{i \leq k+q \\ l \leq j+1-q}} \hat{\sigma}_i^3 \hat{\sigma}_l^3 \Bigg] \hat{\sigma}_j^{q+1}$$

where $\hat{\sigma}_k^1, \hat{\sigma}_k^2, \hat{\sigma}_k^3$ denote the Pauli operators associated with site $k = 1, ..., n$, equivalent with the fermionic Hamiltonian

$$H = \sum_{j,k=1}^{n} \left[\hat{a}_j^{\dagger} A_{j-k} \hat{a}_k + \hat{a}_j^{\dagger} B_{j-k} \hat{a}_k^{\dagger} - \hat{a}_j B_{j-k} \hat{a}_k \right]$$

The fermionic operators obey $\{\hat{a}_j, \hat{a}_k\} = 0$ and $\{\hat{a}_j^{\dagger}, \hat{a}_k\} = \delta_{j,k}$. The Hamiltonians are related via a Jordan-Wigner transformation leading to the Hermitian Majorana operators, $\hat{m}_{2i-1} = (\prod_{j<i} \hat{\sigma}_j^3) \hat{\sigma}_i^1$ and $\hat{m}_{2i} = (\prod_{j<i} \hat{\sigma}_j^3) \hat{\sigma}_i^2$, where $\hat{a}_j = (\hat{m}_{2j-1} - i\hat{m}_{2j})/2$. Translational invariance, periodic boundary conditions, and Hermicity are inherited by $A_j, B_j \in \mathbb{R}$ satisfying $A_j = A_{-j}$, and $B_j = -B_{-j}$ for $j = 1-n, ..., n-1$. For simplicity, we assume that there exists a $w \in \mathbb{N}$ such that $A_j = B_j = 0$ for $j > w$. This model will be our starting point. For all isotropic instances, and also for the full XY model we will be able to identify when the single-copy entanglement is indeed logarithmically divergent. Then, one may distill a maximally entangled state of any dimension from a single specimen of the chain with certainty, containing in this sense an "infinite single-copy entanglement" [25]. We will make use of the powerful methods of Toeplitz determinants [7, 8, 18]. This path is yet in our instance complicated by the fact that we do not only consider isotropic models, and that in contrast to the block entropy the largest eigenvalue cannot straightforwardly be expressed as an integral of a Toeplitz determinant. The starting point, yet, is the familiar one for assessing spin systems: The ground state of this system is a fermionic Gaussian, i.e., quasi-free, state and is completely specified by the second moments of the Majorana operators. These operators satisfy $\hat{m}_j = \hat{m}_j^{\dagger}$ and $\{\hat{m}_j, \hat{m}_k\} = 2\delta_{j,k}$. The second moments can be collected in a correlation matrix $\gamma \in \mathbb{R}^{2n\times 2n}$, $\mathrm{tr}[\rho \hat{m}_j \hat{m}_k] = \delta_{j,k} + i\gamma_{j,k}$. This matrix is skew-symmetric. The entanglement properties of the block of length L can now be inferred from a principal submatrix $\gamma_L \in \mathbb{R}^{2L\times 2L}$ of the correlation matrix γ. We consider the entries of γ_L in the limit of an infinite chain $n \to \infty$. Then, γ_L is a block Toeplitz matrix, the l-th row, $l = 1, ..., L$, being given by $(M_{l-1}, M_{l-2}, ..., M_0, ..., M_{l-L})$, with 2×2-blocks $M_{L-1}, ..., M_{1-L}$ that are found to be

$$M_l = \begin{bmatrix} 0 & t_l \\ -t_{-l} & 0 \end{bmatrix}, \ t_l = \frac{1}{2\pi} \int_0^{2\pi} g(k) e^{-ilk} dk.$$

For no anisotropy, i.e., $B_j = 0$ for all j, this matrix is a tensor product of a symmetric matrix and a unit skew-symmetric one. In generality, we have for this model, $g(k) := \Lambda(k)/|\Lambda(k)|$, $\Lambda(k) := A_0 + 2\sum_{j=1}^{w} A_j \cos(jk) - 4i \sum_{j=1}^{w} B_j \sin(jk)$. This matrix γ_L can be brought into a standard normal form Γ_L of a skew-symmetric matrix with an $O \in O(2L)$ preserving the anticommutation relations,

$$\Gamma_L = O\gamma_L O^T, \ \Gamma_L = \bigoplus_{l=1}^{L} \begin{bmatrix} 0 & \mu_l \\ -\mu_l & 0 \end{bmatrix}.$$

This defines the quantities $\mu_1, ..., \mu_L \in [0, 1]$. Such normal mode decompositions have been employed both to evaluate correlation functions [18] and the block entropy [6, 7, 8]. From now on we will be concerned with the largest eigenvalue of the reduction of a block of length L. All eigenvalues $\alpha_1^{\downarrow}, ..., \alpha_{2^L}^{\downarrow}$ of the reduction are given by $\{\alpha_1^{\downarrow}, ..., \alpha_{2^L}^{\downarrow}\} = \{\prod_{l=1}^{L} (1 \pm \mu_l)/2\}$. We will be looking at the behavior of the largest eigenvalue $\alpha_1^{\downarrow}$ for large L. This largest eigenvalue is given by $\alpha_1^{\downarrow} = \prod_{l=1}^{L} (1/2 + \mu_l/2)$, or

$$\alpha_1^{\downarrow} = \det[(\mathbb{1}_L + |T_L|)/2],$$

$|T_L| = (T_L^T T_L)^{1/2}$, where T_L is the $L \times L$ Toeplitz matrix, with l-th row being given by $(t_{-l+1}, t_{-l+2}, ..., t_0, ..., t_{L-l})$. The numbers $\mu_1, ..., \mu_L$ are the singular values of T_L. This matrix T_L, satisfying $|T_L| \leq \mathbb{1}_L$, is generally not symmetric,

as a consequence of the anisotropy of the model. Moreover, in contrast to the matrix T_L itself, $\mathbb{1}_L + |T_L|$ is not Toeplitz. In order to show that the single-copy entanglement is logarithmically divergent, we will make use of appropriate bounds that retain this property: whenever the $A_0, ..., A_w$, $B_0, ..., B_w$ are such that one can prove that the sequence of $L \times L$-Toeplitz matrices T_L satisfies

$$-\log|\det[T_L]| = \Omega(\log(L)) \tag{2}$$

(using Landau notation [20]) using a Fisher-Hartwig-statement [7, 8, 18], then one can indeed conclude that $E_1 = \Omega(\log(L))$, i.e, the single-copy entanglement diverges at least logarithmically with increasing block length L. This follows from the following chain,

$$\begin{aligned}- &\log\det[(\mathbb{1}_L + |T_L|)/2] \geq -\frac{1}{2}\log\det[(\mathbb{1}_L + T_L^T T_L)/2] \\ \geq &-\frac{1}{4}\log\det[T_L^T T_L] = -\frac{1}{2}\log|\det[T_L]|\end{aligned}$$

[27], where we also have made use of the concavity of the logarithm. So, whenever Eq. (2) holds, for appropriate length of the block L, a maximally entangled pair of any dimension can be distilled from a single specimen of the spin chain.

Isotropic models. – This case of $B_0, ..., B_w = 0$ is particularly transparent. Here, the asymptotics in L of the determinants $\det[M_{x,L}]$ of the $L \times L$-Toeplitz matrices $M_{x,L} := ix\mathbb{1} + (1-x^2)^{1/2}T_L$ is known for all $x \in (0,1)$, using a Fisher-Hartwig statement. This small detour to infer about $-\log|\det[T_L]|$ – corresponding to the case $x = 0$ – is needed as the Fisher-Hartwig-conjecture has not been proven yet for this case. In general, one can identify the asymptotic behavior of determinants of Toeplitz matrices by investigating the so-called symbol, see footnote [21]. The symbol associated with the Toeplitz matrices $M_{x,L}$ is given by

$$G_x(k) = ix + (1-x^2)^{1/2}g(k),$$

with g as defined above. For this class of isotropic models, an explicit factorization of the symbol is known [8], see footnote [22]. It follows hence from proven instances of the Fisher-Hartwig conjecture that there exists a $c > 0$ and an $x_0 \in (0,1)$ such that [20]

$$\log|\det[M_{x,L}]| = c_x \log(L) + o(\log(L))$$

with $c_x > c$ for all $x \in (0, x_0)$, whenever the function g is discontinuous in $[0, 2\pi]$, where the jumps reflect the Fermi surface. From this – and using that T_L has real eigenvalues – it follows that the system has a logarithmically divergent single-copy entanglement if the system is critical [23]. For example, for the XX model this analysis immediately delivers a logarithmically divergent single-copy entanglement, whenever the system is critical.

Anisotropic XY-model. – For the XY-model we can conclude that the single-copy entanglement is logarithmically divergent if and only if the system is critical. For this model, we have that $A_0 = -1, A_1 = a/2$ and $B_{-1} = -B_1 = \gamma a/4$, and 0 elsewhere. For $\gamma = 0$, we obtain the XX-model (the isotropic XY-model), for $a = 1$, $\gamma = 1$ the critical Ising model. Along the line $\gamma \in [-1,1]$, $a = 1$ the anisotropic model is critical. Then, we encounter a generally non-symmetric matrix T_L. The associated symbol is given by

$$g(k) = \frac{a\cos(k) - 1 + ia\gamma\sin(k)}{((a\cos(k)-1)^2 + \gamma^2 a^2 \sin^2(k))^{1/2}}.$$

For $\gamma \neq 0$ and $1/a \in (0,1)$, the symbol is continuous, and one finds a saturating block entropy [7] (and hence a saturating single-copy entanglement). Along the critical line $a = 1$, $\gamma \in (-1,1)$, in turn, we can identify the explicit factorization of the discontinuous symbol. There is a single discontinuity at $k_1 = 0$ [28], and in the terms of footnote [22] we find $\beta_1 = 1/2$, so that $g(k)$ can be decomposed as

$$g(k) = \phi(k) t_{1/2}(k),$$

where ϕ is a continuously differentiable function. For the case of a single discontinuity and $\alpha_1 = 0$, the Fisher-Hartwig conjecture has been proven for any $\beta_1 \in \mathbb{C}$ with $\Re(\beta_1) < 5/2$ [19], including our case at hand. Hence, we find $-\log|\det[T_L]| = \Omega(\log(L))$, and hence $E_1 = \Omega(\log(L))$. Together with the result of the subsequent section this shows that the single-copy entanglement of the XY-model is logarithmically divergent exactly if the model is critical. Note that this implies also a less technical alternative proof of the logarithmic divergence of the block entropy in the critical XY model.

Scaling of single-copy entanglement in the XX-model. – In the light of these findings, it is interesting to see how the exact asymptotic behavior is compared to that of the block entropy, including prefactors. We make this specific for the isotropic XX-model, where now $T_L = T_L^T$. The technicality when evaluating $\alpha_1^{\downarrow} = \det[(\mathbb{1}_L + |T_L|)/2]$ that we encounter here is that the function $f : \mathbb{C} \to \mathbb{C}$, $f(x) := \log_2((1+|x|)/2)$, is not analytic. So before we can exploit Fisher-Hartwig-type results, we have to approximate $\alpha_1^{\downarrow}$ with sequences based on functions with appropriate continuity properties. We can take any functions $f_* : \mathbb{C} \times \mathbb{R}_+ \to \mathbb{C}$ which are analytic on $\{z \in \mathbb{C} : \Im(z) < \delta\}$ for a $\delta > 0$, such that on the real axis $\lim_{\delta \searrow 0} f_*(x,\delta) = f(x,0)$ for $x \in \mathbb{R}$. Take, e.g.,

$$f_*(z,\delta) := \log(1/2 + (z^2 + \delta^2)^{1/2}/2).$$

We are then in the position to identify the asymptotic behavior of the single-copy entanglement. This can be done similarly to Ref. [7] using the characteristic polynomial $F : \mathbb{C} \to \mathbb{C}$ of T_L defined as $F(\lambda) := \det[\lambda\mathbb{1}_L - T_L]$: the function F is meromorphic, and all zeros are in the interval $[-1,1]$. One can hence write

$$d_* = \lim_{\delta \searrow 0} \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \int dz f_*(z,\delta) \frac{F'(z)}{F(z)} \tag{3}$$

where the integration path is chosen to enclose the interval $[-1,1]$, with path from $(-1-\delta+i\varepsilon, 1+\delta+i\varepsilon)$, towards the negative real numbers along a circle segment with radius

$\delta/2$, then $(1+\delta-i\varepsilon, -1-\delta-i\varepsilon)$, and again along a circle segment to $-1-\delta+i\varepsilon$, such that $\lim_{\delta\searrow 0} d_* = d$. The symbol of $\lambda\mathbb{1} - T_L$ with factorization as in Eq. (4) for the XX-model is known [7], see footnote [22]. Using a Fisher-Hartwig statement, we find that the linear terms in L do not contribute, using Cauchy's theorem and using that $\lim_{\delta\searrow 0} f_*(\pm 1, \delta) = 0$, and finally arrive at

$$d = \log(L)\frac{2}{\pi^2}\int_{-1}^{1}\frac{\log_2[(1+|x|)/2]}{1-x^2}dx + o(\log(L)).$$

This in turn finally implies that whenever $1/a \in [-1,1]$ and the XX-model is critical, we observe the scaling behavior

$$E_1 = \frac{1}{6}\log_2(L) + o(\log(L)),$$

independent of a; it saturates in the non-critical case. This result is astonishing: the single-copy entanglement does not only diverge, but has up to a factor of two the same asymptotic behavior as the entropy of entanglement scaling as $S = (1/3)\log_2(L) + o(\log(L))$. Half of the asymptotically distillable entanglement is hence already available on the single-shot level.

Outlook and summary. – Finally, let us comment on the crucial role of SSR for the single-copy entanglement. This is relevant, e.g., when assessing the single-copy entanglement in the hard-core limit of the Bose-Hubbard model (infinite repulsion energy) [1]. There, the Hamiltonian is isomorphic to the XX-model, via the mapping $\hat{\sigma}^1_j = \hat{b}_j + \hat{b}^\dagger_j$, $\hat{\sigma}^2_j = -i(\hat{b}_j - \hat{b}^\dagger_j)$, and $\hat{\sigma}^3_j = 1 - 2\hat{b}^\dagger_j\hat{b}_j$ for each site j. Yet, the concept of entanglement is different due to the presence of a particle number conservation SSR in the former case: Transformations under LOCC have to be replaced by those under LOCC+SSR. The single-copy entanglement in the above sense can however still be efficiently evaluated in L; and these superselection rules must be respected when assessing single-copy entanglement.

In this paper, we have fleshed out the notion of single-copy entanglement in quantum spin chains. Such a notion is the appropriate one when one is not interested in the entanglement properties of an asymptotic supply of a identically prepared many-body systems, but of single specimens. It is the hope that these findings also serve as a guideline when assessing entanglement in actual experimental situations, let it be in condensed-matter systems or in systems of ultracold atoms in optical lattices.

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[20] For functions of L, $f = O(g)$ means that $f \leq cg$ for some $c > 0$ and all L, $f = o(g)$ means that $f/g \to 0$ for $L \to \infty$, and $f = \Omega(g)$ that $f \geq Cg$ for some $C > 0$ and all L.

[21] For an square summable sequence $\{s_k\}_k$, $s_k \in \mathbb{C}$, the symbol G corresponding to a sequence of $L \times L$ Toeplitz matrices with l-th row $(s_{l-1}, ..., s_{L-l})$ is given by $G(k) = \sum_{j=-\infty}^{\infty} e^{ijk} s_j$.

[22] For this class of isotropic models, an explicit factorization of the symbol is given by

$$\begin{aligned} G_x(k) &= -(1-x^2)^{1/2} h(x)^{\sum_{r=1}^{R}(-1)^r k_r/\pi} \\ &\times \prod_{r=1}^{R} t_{(-1)^r f(x)}(k-k_r) t_{-(-1)^r f(x)}(k+k_r), \end{aligned} \quad (4)$$

$t_\beta(k) := \exp(-i\beta(\pi - k \mod 2\pi))$, $h(x) := (ix - (1-x^2)^{1/2})/(ix + (1-x^2)^{1/2})$ and $f(x) := (\log \circ h)(x)/(2\pi i)$. k_r, $r = 1, ..., R$, are the k for which g is discontinuous.

[23] Here, we use critical in the sense that there is no gap between the energy of the ground and the first excited state.

[24] Here, for $x = |x|e^{i\varphi} \in \mathbb{C}\backslash\{z \in \mathbb{C} : \Im(z) = 0, \Re(z) < 0\}$ we take $\log(x) = \log|x| + i\varphi$.

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